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Freckle Formation in IN718 Under Vertical and Tilted Growth Conditions

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Abstract. In industrial processes involving molten metals, freckles are a common defect in nickel-based superalloy castings, which negatively impact mechanical performance. Castings with freckles are often discarded, leading to significant economic losses, as these defects cannot be eliminated through post-casting or thermomechanical treatments. Despite advancements in understanding the mechanisms behind these defects, reliable theories and empirical guidelines to inform engineering design remain scarce. This study investigates the formation of segregated channels during the directional solidification (DS) of Ni-5wt%Nb alloy, focusing on the influence of growth front inclination on macro-segregation and solute-driven convection. A two-phase solidification model, coupled with fluid flow, heat transfer, and solute transport, is employed to simulate the solidification of Ni-5wt%Nb alloy in a 3D cylindrical geometry with a diameter of 25 mm and a length of 150 mm using the finite volume method. Two cases are considered: (i) vertical solidification (0° tilt) and (ii) inclined growth (35° tilt) to replicate the experimental conditions reported by Auburtin et al. [Met and Mat Trans B, 2000]. The results demonstrate that no segregated channels form in the vertical solidification case, whereas segregated channels appear in the 35° tilt case, aligning with experimental observations. The analysis of segregation maps confirms that the inclined growth front enhances solutal convection, leading to the formation of segregated channels. A comparison with a published experimental setup, which closely resembles the classical Bridgman furnace used in industry, demonstrates good agreement with the simulation results.

1. Introduction

Nickel-based superalloys, such as Inconel 718 (IN718), are extensively utilized in aerospace, power generation, and other high-temperature applications due to their superior mechanical properties, oxidation resistance, and creep strength. DS is a widely employed casting technique that enhances the microstructural control of these alloys, improving their mechanical performance under extreme conditions. However, defects such as freckles, a form of macro-segregation-pose significant challenges in the production of high-quality castings. Freckles manifest as segregated, solute-enriched channels aligned with the primary solidification direction, leading to localized variations in composition that deteriorate mechanical properties and component reliability [1-3]. Freckling arises from solutal buoyancy-driven convection in the

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mushy zone, where interdendritic liquid enriched in solute elements becomes less dense and ascends, forming stable segregated channels. These defects are particularly prevalent in nickel-based superalloys due to their complex multi-component chemistry and the pronounced effect of segregation on phase stability. The formation of freckles is governed by key parameters such as the Rayleigh number, cooling rate, and the solidification front geometry [4]. Despite extensive experimental and numerical investigations, the prediction and mitigation of freckles remain challenging, as their formation is influenced by multiple factors, including thermal gradients, cooling rates, and alloy composition. Since freckles cannot be effectively removed through post-processing or thermomechanical treatments, their presence often results in significant material loss and increased manufacturing costs [5]. Several studies have contributed to advancing the understanding of freckle formation. Auburtin et al. [5] proposed a freckle criterion based on the interaction between buoyancy-driven flow and dendritic solidification in superalloy castings. More recently, Liu and Wang [6] introduced a geometric-based freckle prediction model, improving defect forecasting in complex-shaped components. Furthermore, Wang et al. [4] used advanced electron microscopy to validate the convection-induced freckle formation theory, reinforcing the role of thermosolutal convection in the segregation process.

To gain deeper insight into the formation of the segregated channels phenomenon, this study presents a numerical investigation of segregated channels formation during the DS of Ni-5wt%Nb alloy. A two-phase solidification model is employed to simulate the coupled effects of heat transfer, fluid flow, and solute redistribution in a three-dimensional (3D) cylindrical domain using the finite volume method. The model captures key transport phenomena, including thermo-solutal convection, buoyancy-driven flow, and macro-segregation, providing a detailed analysis of the conditions leading to segregated channels formation. The results are validated by comparing simulation outputs with experimental data obtained from a Bridgman-type DS furnace, including the study by Auburtin et al. [5], which serves as a reference for the experimental setup.

2. Model description

A three-dimensional (3D) two-phase mixture model has been developed to investigate the formation of segregated channels during the DS of Ni-5wt%Nb. The two phases represent the liquid melt (primary phase) and the solid dendritic (secondary phase), quantified by their respective volume fractions, f_l, and f_s. These fractions sum to unity, expressed as: $f_l + f_s = 1$. The solid phase is assumed stationary, i.e. $u_s = 0$; while the motion of the fluid is calculated by solving the momentum conservation equation, incorporating buoyancy-driven convection and flow resistance in the mushy zone. The numerical simulation is conducted in a cylindrical domain consisting of 25 mm diameter and 150 mm length, replicating the Bridgman-type furnace setup from Auburtin et al. [5]. The bottom cooling, which corresponds to the casting-spacer interface, is assigned an effective heat transfer coefficient (HTC) of 200 W/m^2·K with exterior temperature equals to 873K, as determined by Auburtin et al. (2000) using the PROCAST model. These values account for the presence of a spacer between the casting and the chill plate, leading to moderate heat extraction that ensures DS while avoiding excessive cooling. Similarly, the side walls, which were in contact with an alumina mold, are assigned an HTC of 50 W/m^2·K, also based on the PROCAST model predictions from Auburtin et al. (2000). This sidewall cooling induces radial solidification, which interacts with the vertical growth front, influencing the shape of the dendritic network and the formation of macro-segregation patterns. In the simulation, the hot and cold zones are reproduced through boundary conditions. The entire domain is initially above the liquidus temperature, and cooling is applied from the bottom and side walls. This causes the

bottom and sides to act as the cold zone, while the top remains hot due to the absence of cooling, consistent with the experimental setup. In addition, all boundaries of the casting domain were treated as no-slip walls. The volume-averaged conservation equations for mass, momentum, species, and enthalpy are solved for the mixture phase. The model has been described in detail elsewhere [7, 8], except the drag force, which was solved using the Carman Kozeny function (equation 1), which is defined as a function of the secondary dendrite arm spacing λ_2, as follows:

$$\vec{F}_{Darcy} = \mu \frac{f_l}{K} \vec{u}_l, \text{ with } K = \frac{\lambda_2^2 f_l^{\,3}}{180 f_s^{\,2}} \tag{1}$$

Here, K is the permeability, μ is the viscosity, and $\vec{u}_l$ is the liquid velocity. The thermophysical properties of the Ni-5wt%Nb alloy are given elsewhere, [9]. The simulation is implemented in a finite volume framework to simulate the solidification of Ni-5wt%Nb alloy. Buoyancy-driven flow is modeled using the Boussinesq approximation, in which density variations due to temperature and concentration are included only in the body force (gravity) term of the momentum equation. However, the density was considered constant elsewhere in the governing equations, as defined in [7]. In this study, two cases of DS are simulated to investigate the influence of the growth front orientation on segregated channels formation, replicating the experimental conditions reported by Auburtin et al. [5]. The first case considers a vertical growth direction (0° tilt angle), where the casting remains upright and the solidification front advances predominantly upward. The second case simulates a tilted growth condition (35° tilt angle), where the casting is inclined relative to the vertical axis, modifying the buoyancy-driven flow within the mushy zone. In our simulation of tilted directional solidification, the tilt is applied to the casting geometry. However, the gravity vector remains aligned with the vertical direction (i.e., pointing downward, normal to the Earth's surface). The thermal boundary conditions were kept identical between the vertical and tilted cases, consistent with the experiment. The thermal gradient in the simulation is therefore not artificially tilted; rather, it develops naturally through heat extraction from the bottom and side walls of the inclined casting. The simulation reproduces the experimental setup by adopting the same casting geometry and applying boundary conditions equivalent to those used in the experiment. The alloy IN718-Si was approximated using a Ni-5wt%Nb binary system to preserve the dominant segregation behavior relevant to freckle formation and to reduce computational complexity. This approximation is commonly used in solidification modeling studies to capture the key solute redistribution and macro-segregation behavior of IN718, as demonstrated in previous works [9, 10]. The substitution of the multicomponent IN718-Si alloy with a Ni-5wt%Nb model allows for a more focused analysis of solutal convection and freckle formation, as Nb is the primary segregating element responsible for macro-segregation in IN718-Si.

To accurately capture the thermal and solutal transport phenomena during the DS of Ni-5wt%Nb, a structured O-grid mesh was employed consists of 720,000 elements, ensuring a high level of spatial accuracy while maintaining computational efficiency. By maintaining these thermal boundary conditions, the simulation ensures a realistic comparison with the experimental data, allowing for an in-depth analysis of thermal and solutal convection and their role in segregated channels formation under different growth orientations. The two cases will allow us to quantify the effect of growth front inclination on the onset and severity of macro-segregation defects, providing insights into how process conditions influence freckle formation in nickel-based superalloys.

3. Results and discussions

3.1 Evolution of the solidification front

The evolution of the solid fraction during the DS of Ni-5wt%Nb alloy is presented in Figure 1, which shows the progression of solidification for Case 1 (0° tilt) and Case 2 (35° tilt) at five instants: t=200, 300, 600, 1000, and 1100 s. As expected, solidification initiates at the bottom of the casting, where the highest heat transfer coefficient (HTC) is applied, and progresses upward as the heat is extracted. At early time instants (t=200-300 s), solidification in both cases follows a bottom-to-top direction, with the formation of a mushy zone where dendrites grow as the temperature decreases below the liquidus temperature. However, the solidification front remains uniform and horizontal in the vertical case, reflecting symmetric thermal and solutal conditions. In contrast, the tilted case shows a clearly inclined (marked by ΔH) and distorted front, caused by asymmetrical solutal convection due to the misalignment between gravity and the solidification direction. Solidification progresses faster from the bottom than the sides due to stronger cooling at the bottom surface, while the lower heat transfer at the side walls (HTC = 50 W/m²·K) leads to
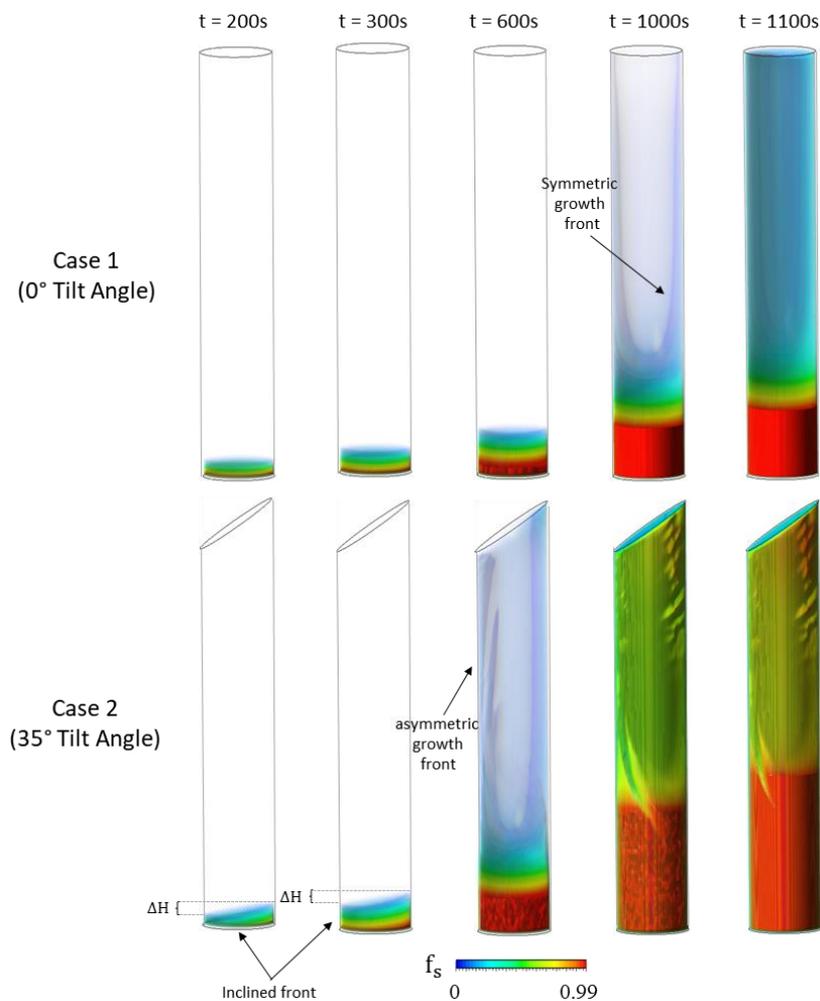

Figure 1. Solid-liquid front position at different instants during the solidification of Ni-5wt%Nb alloy. The top row is case 1 with a 0° tilt angle, and the bottom row is case 2 with a 35° tilt angle.

slower radial solidification. This thermal asymmetry results in a curved solidification front and influences the mushy zone development. Additionally, solidification in the tilted case occurs faster than in the vertical case, as observed at t=600s t=600s, where the side walls of the tilted geometry begin to solidify, while in the vertical case, solidification at the side walls begins only at t=1000s. Although the boundary conditions are identical in both cases, the tilted geometry enhances local heat extraction due to the orientation of the sidewalls relative to the thermal gradient and the development of asymmetric buoyancy-driven flow. These effects bring cooler regions into earlier contact with the melt along the lower inclined wall, promoting more efficient heat removal and initiating sidewall solidification earlier than in the vertical case. At t=1100s, the vertical case shows a uniform solidified structure with the last remaining liquid region located in the upper central area, indicating a stable and symmetric solidification front. In contrast, the tilted case still contains partially liquid regions where segregated channels are developing. These zones remain in a liquid state longer due to Nb enrichment and buoyancy-driven solutal convection, highlighting the influence of growth front inclination on delaying local solidification and promoting segregated channels formation.

3.2 Effect on segregation

The simulation results illustrating the evolution of segregation patterns during the solidification in both the vertical (Case 1) and tilted (Case 2) configurations are presented in Figure 2, captured at five different time instants. Indeed, the segregation structures shown in Figure 2 correspond to regions of positive segregation, where the local solute concentration exceeds the nominal alloy composition. At the early stage of solidification (t = 200-300 s), the segregation differences in both cases are minimal, as solidification has just initiated and solutal convection remains weak. As the process progresses (t = 600 s), segregated channels formation becomes clearly visible in the tilted case, where multiple upward solute plumes begin to develop within the mushy zone. These segregated channels are noticeably inclined, aligning with the direction of the solute-driven buoyancy flow, which is influenced by the tilted geometry. Unlike the vertical case, where flow structures remain more symmetric, the tilted configuration introduces asymmetric convection patterns that destabilize the mushy zone and promote the emergence of solute-enriched channels at an angle. The numerical model predicts the development of solute-enriched segregated channels, which are considered precursors to freckle formation based on experimental observations. This inclination of the segregated channels reflects the influence of both gravity and the inclined solidification front, resulting in directional solute transport that favors segregated channels growth along an oblique path. The segregated channels become more pronounced at later times, such as t = 1000 s and beyond. However, no segregated channels were observed in the vertical case. Overall, these findings are in strong agreement with the experimental results reported by Auburtin et al. [5], where freckles were also observed only in the tilted configuration, confirming the critical role of growth front orientation in freckle formation.

Figure 3 presents a comparison between the experimental and simulated results for the final macrosegregation state in both solidification cases. In the simulation, the visible regions correspond to areas of positive segregation, where the local Nb concentration exceeds the initial alloy composition (note that the minimum value of the color scale represents the nominal 5 wt% Nb). For the 0° tilt case, no segregated channels are observed in the experimental sample, consistent with the simulated distribution. While the simulation shows a slight solute variation (only 0.02 wt%Nb), the degree of segregation is minimal, resulting in more uniform segregation, confirming the overall stability of the solute transport under vertical solidification conditions. In
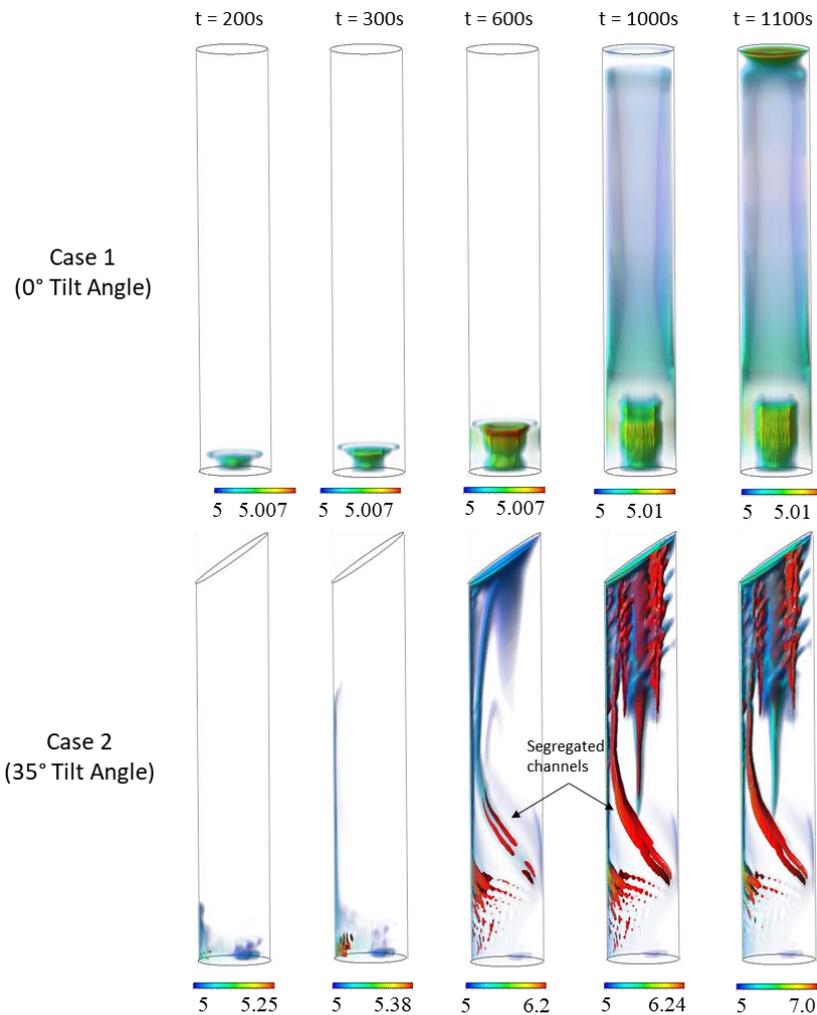
Figure 2. Segregation structures at different instants during the solidification of Ni-5wt%Nb alloy. The top row is case 1 with a 0° tilt angle, and the bottom row is case 2 with a 35° tilt angle.

contrast, the 35° tilt case exhibits pronounced segregated channels in both the experiment and the simulation. The simulation reveals well-defined segregated channels, where the Nb concentration locally exceeds the nominal value by up to 2 wt%Nb. This strong solutal variation arises from enhanced buoyancy-driven flow triggered by the inclined solidification front, which promotes solute convection and instability within the mushy zone. While our simulation successfully captures the overall trend observed in the experiments, the morphology and distribution of the simulated segregated channels differ from those seen experimentally. This discrepancy arises primarily from the simplified alloy model used in the simulation: the experiment was conducted with IN718-Si, while our model is based on a Ni-5wt%Nb binary approximation, which lacks the full complexity of multicomponent segregation. Moreover, key thermophysical parameters, such as the solutal expansion coefficient, were estimated rather than calibrated for the experimental alloy. Despite these limitations, our results align well with the experimental study by Auburtin et al. [5], confirming the critical influence of growth front inclination on solutal convection and macrosegregation behavior.
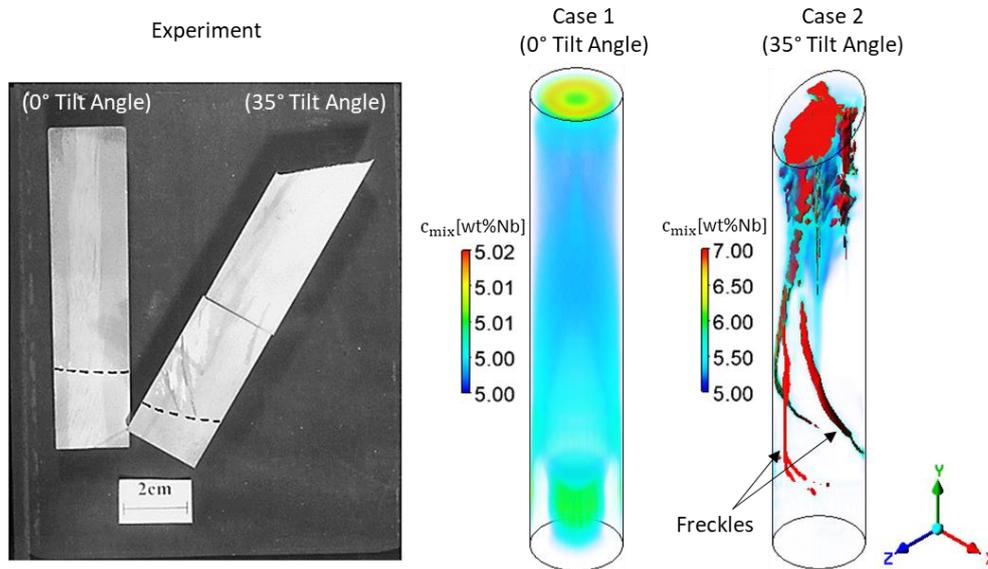
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Figure 3. Experiment (left) presents the typical DS samples cast at 0 and 35 degrees to the vertical, [5], and simulation (middle and right) results present the final macrosegregation developed.

Combeau et al. [2,3] and Saad et al. [11] have demonstrated that channel formation can occur even under vertically aligned solidification conditions, depending on the strength of solutal convection and local instability criteria. In our work, inclination is not the sole criterion for segregated channels formation, but rather that it is a dominant destabilizing factor under the specific thermal and geometrical conditions of our study, which aims to replicate the experimental setup of Auburtin et al. [5]. In the vertical (0°) case, buoyancy-driven flow is fully resolved in 3D, and instabilities are allowed to develop naturally. The velocity field was carefully examined and showed that upward flow remained weak and relatively uniform throughout the mushy zone, suppressing solute plume formation. The absence of visible channels in this case is therefore likely due to the combined effect of alloy properties (Ni–5wt%Nb), solutal convection, and applied thermal boundary conditions, which result in weaker convection. While our results highlight the influence of growth front inclination. In contrast, other parameters such as Rayleigh number, alloy composition, and cooling can also drive channel formation in vertically solidified alloys, as demonstrated in previous works [2, 3, and 11]. This validates the predictive capability of our numerical model and provides valuable insight for optimizing casting processes in nickel-based superalloys, where controlling the orientation of the solidification front can effectively suppress freckle defects and enhance the performance and reliability of components in aerospace and power generation applications.

Conclusion

This study presents a comprehensive numerical investigation of segregated channels formation during the DS of Ni-5wt%Nb alloy, focusing on the influence of growth front inclination on macrosegregation and solute-driven convection. Using a two-phase solidification model implemented in a finite volume framework, we simulated the evolution of the mushy zone, solidification front, and solute segregation patterns under two distinct conditions: a vertical

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growth front (0° tilt) and a tilted front (35° tilt). The results show that while the vertical case remains free of segregated channels, the tilted configuration exhibits pronounced freckling, which was in good agreement with experimental observations reported by Auburtin et al. [5]. The findings highlight the key role of growth front geometry in destabilizing solutal convection and promoting freckle-prone flow channels, particularly in alloys with strong segregation behavior such as Ni-5wt%Nb. The enhanced freckling in the tilted case is attributed to the asymmetric interaction between buoyancy-driven flow and the inclined dendritic structure. By capturing these complex interactions, the model not only validates experimental tendencies but also offers critical insight into how process conditions can be optimized to suppress freckle formation. This work contributes to the broader understanding of macrosegregation phenomena in superalloy castings and supports the development of more reliable manufacturing strategies for high-performance components in the aerospace and power generation industries.

Acknowledgments

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